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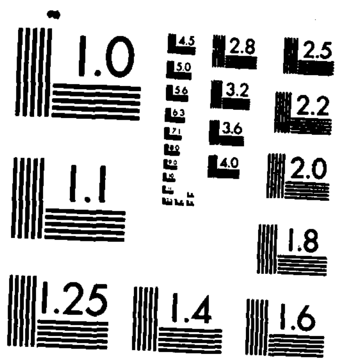

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"NUMERICAL SIMULATION OF TURBULENT FLAMES USING VORTEX METHODS"

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SUMMARY

Vortex schemes for direct numerical simulation of turbulence are developed to study the propagation and stability of turbulent flames. Attention is focused on the construction of accurate and efficient computational algorithms that are easily extendable to three dimensional reacting flow at high Reynolds numbers. A Lagrangian vortex scheme, which incorporates stochastic simulation of diffusion, was used to obtain solutions for a recirculating flow and a mixing layer. Results showed good agreement with experimental data at intermediate Reynolds number for the first case, and was used to establish the convergence of the numerical method, the sources of errors and the appropriate scheme to improve the accuracy efficiently. For the mixing layer, the simulation predicted the average velocity and the streamwise fluctuations accurately, but overpredicted the cross-stream fluctuation, indicating that the latter are governed by the three dimensional effects. The response of the layer to harmonic modulations was analyzed revealing the nature of the flow and indicating how entrainment can be enhanced in shear flow. The relationship between the flow instability and the combustion stabilization in both cases indicated the premixed flames have a narrow range of stable existence in terms of the equivalence ratio.

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

SUMMARY - Vortex schemes for direct numerical simulation of turbulence are developed to study the propagation and stability of turbulent flames. Attention is focused on the construction of accurate and efficient computational algorithms that are easily extendable to three dimensional reacting flow at high Reynolds numbers. A Lagrangian vortex scheme, which incorporates stochastic simulation of diffusion, was used to obtain solutions for a recirculating flow and a mixing layer. Results showed good agreement with experimental data at intermediate Reynolds number for the first case, and was used to establish the convergence of the numerical method, the sources of errors and the appropriate scheme to improve the accuracy efficiently. For the mixing layer, the simulation predicted the average velocity and the streamwise fluctuations accurately, but overpredicted the cross-stream fluctuation, indicating that the latter are governed by the three dimensional effects. The response of the layer to harmonic modulations was analyzed revealing the nature of the flow and indicating how entrainment can be enhanced in shear flow. The relationship between the flow instability and the combustion stabilization in both cases indicated the premixed flames have a narrow range of stable existence in terms of the equivalence ratio.

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RESEARCH OBJECTIVES

In this research program, methods for direct numerical simulation of turbulence are developed to study combustion in turbulent shear flow. Time-dependent solutions of the Navier-Stokes equations for a reacting mixture are obtained using vortex schemes. Attention is focused on problems of flame propagation at low Mach numbers and turbulent flame stabilized in confined mixing layer and recirculating flow. In particular:

(1) Constructing a two-dimensional solution for a confined mixing layer, a recirculating flow, and a cavity flow, and comparing the numerical results with experimental data in terms of average velocity profiles, average turbulent statistics, and the pressure field;

(2) Establishing the limits of application of two-dimensional models for shear flow;

(3) Extending the numerical scheme to account for three-dimensional phenomena by modifying the two-dimensional random vortex method to include stretching and tilting of vorticity;

(4) Incorporating the thin flame model into the turbulent flow solution and comparing the numerical results with the experimental data;

(5) Defining the range of stability of turbulent flames in premixed gases in terms of the mixture equivalence ratio, the Reynolds number and inlet flow conditions;

(6) Using the developed methodology to improve the understanding of the mechanism of stability of turbulent flames.

PERSONNEL

Besides the principal investigator, five graduate students and one undergraduate student are currently supported, either partially or fully, by this grant. Their names, degree objective and starting dates are:

1.	Gagnon, Yves	M.Sc. (in progress)	September 1984
2.	Knio, Omar	M.Sc. (in progress)	September 1984
3.	Ng, Kenneth	M.Sc. (in progress)	January 1985
4.	Heidarinejad, Ghassem	Ph.D. (in progress)	January 1985
5.	Samarasan, Dhanesh	B.Sc. (in progress)	June 1985
6.	Najm, Habib	Ph.D. (in progress)	September 1985

EQUIPMENT

In the first phase of the project, the following facility has been established to perform the necessary computations:

(1) VAX-11/750 CPU with 3Mbytes and a FP75.

This machine is used for code development, small batch computing, pre- and post-data processing, graphics and word processing.

(2) An array processor.

This unit increases the computational speed of the VAX by an order of magnitude, making it possible to run medium batch processes.

(3) Permanent communication capability.

For interaction with a supercomputer (CRAY type), to be used for long batch computing when time is available on either NSF Supercomputing centers, through DOD or NASA support.

STATUS OF RESEARCH

The research program has been divided into four topics. A brief description of each project, its current status and the future plans is summarized in the following. Details are described in the accompanying publications.

I. Vortex Simulation of a Confined, Perturbed Shear Layer

Ample experimental evidence has been accumulated for the effect of externally imposed perturbations, in the form of pressure oscillations or organized velocity fluctuations, on the dynamic behavior of the large eddy structures in turbulent shear flow. Pressure modulations can enhance, delay or paralyze the pairing of eddy structures, depending on the frequency and phase relation between the imposed excitation and the natural oscillations of the layer. Since most of the mixing occurs during the pairing process, these modulations can exert a direct influence on mixing-controlled combustion processes that are stabilized in the wake of a shear layer flow. We are studying this process computationally.

In order to predict the natural behavior of a turbulent shear layer, computational results are obtained for a high Reynolds number flow developing behind a splitter plate in a channel. A Lagrangian vortex scheme, which utilizes finite vortex elements to discretize the vorticity field, conformal mapping to implement the potential boundary condition, and random walk to simulate the effect of diffusion (Ghoniem [1]), is used. The results are analyzed in terms of the average velocity profiles and turbulent statistics.

Using a Fast Fourier Transform, the most unstable frequencies of the layer, associated with the formation of the large eddies, are identified

from the numerical output. Results show that the numerical simulation predicts the rate of growth of the layer and the average velocity profiles very accurately. Similar accurate predictions are obtained for the kinetic energy of fluctuations and the Reynolds shear stresses. However, the kinetic energy of fluctuations in the cross stream direction are overpredicted due to the lack of the three dimensional effects in the numerical simualtions. The results of this part of the study is documented in Ng and Ghoniem [2].

The effect of imposing monochromatic perturbation on the velocity of the incoming high-speed stream is currently being investigated using the same scheme. Preliminary results indicate that forcing accelerates the initial growth of the layer, causing the formation of an eddy with a passage frequency equal to the forcing frequency. This is followed by a region in which pairing is inhibited, i.e. forcing at a frequency inhibits its subharmonic. After a number of wavelengths, depending on the forcing amplitude, the effect of forcing decays and the layer resumes its natural growth. We have compiled data for forcing at a number of frequencies and at different amplitudes to generalize these conclusions, and to extend the study to the case of dichromatic forcing, both in- and out-of-phase. The results of this part will be publishd in Ng and Ghoniem [3].

We are planning to use this simulation to study the physics of entrainment and mixing in the shear layer. Of particular interest is the rate of entrainment from the two sides of the layer and the effect of various dynamical parameters, such as the Reynolds number, the shear factor, and the upstream forcing on the rate of mixing of the two streams. This will be the beginning of a study of mixing-controlled combustion in a shear layer, in which particles traced in a Lagrangian frame of reference will be used to represent different species in a chemical reaction process.

II. Low Frequency Oscillation of Recirculating Flows

Recirculating flows represent a more complicated form of shear flows, in which the interaction between the separating shear layer and the recirculation zone can establish favorable conditions for stabilization of combustion. Under conditions of high heat release rates in premixed combustion, these flows exhibit large amplitude, low frequency pressure oscillations that endangers the safety of the combustor. These oscillations have been shown to exist in cold flow at a wide range of Reynolds number and it is suspected that heat release only energizes these oscillations to higher amplitude. Using accurate and efficient numerical predictions of recirculating flows, we are planning to identify the natural frequency of oscillation and examine the behavior of the flow under conditions of upstream forcing.

We have successfully shown that the random vortex method is capable of simulating the recirculating flow behind a rearward-facing step in a channel at a wide range of Reynolds number (Ghoniem and Sethian [4]). Within that range, the dynamics of the flow field changes from viscous-laminar, to transition and early turbulent behavior. The numerical results reveal the changes in the structure of the recirculation zone as viscous forces become dominated by the growth of random perturbations at high Reynolds numbers. The delicate balance between convection and diffusion is thus captured by the numerical simualion.

The accuracy of the numerical prediction is assessed further by comparing the results, in terms of the streamwise velocity profiles, with experimental data at low Reynolds numbers where three dimensional effects are absent. This study required the identification of the sources of errors in the random vortex methods and the design of the appropriate strategy of

controlling these errors by adjusting the numerical parameters effectively. We found that using vortex elements with large values of circulation introduces numerical diffusion that diminshes small negative velocities around the reattachment zone, hence producing smaller recirculation zones than expected. Moreover, since the scheme maintains the velocity at zero along the boundaries, it may produce a large number of "parasitic vortices", i.e. vortices that cancel the effect of strong, highly concentrated vortex elements. Thus, care must be exercised in choosing the maximum allowable strength of elementary vortices in order to control the error and to produce minimum number of vortex elements necessary to represent the vorticity field. The results of this study are being prepared for publication in Gagnon and Ghoniem [5].

The variation of the recirculation zone length with time shows that the flow possesses a natural low frequency that the experimental results had indicated. We are currently computing the time-dependent pressure field and plan to use these results in further investigation of the intrinsic unsteadiness of recirculating flows. The relationship between the dominant frequency and the rate of formation of eddies on the downstream side of the recirculation zone is important in the mixing between the recirculating fluid and the incoming fluid. This relationship will be obtained from the numerical result by performing a spectral analysis on the time-dependent velocity field. Meanwhile, we are planning to compute the distribution of the residence time of passive particles which are injected in the free stream to determine the effectiveness of the recirculation zone in stabilizing a premixed flow. The dependence of the characteristic parameters of this distribution on the Reynolds number will be calculated from our results.

III Spanwise Structure of a Turbulent Shear Layer

Three-dimensional effects, in particular vortex tilting and stretch, become important after the initial stages of development of turbulent shear flow. These effects promote noticeable changes in the dynamics and structure of shear layers, which alter the rates of entrainment between two separate streams and result in "mixing transition." The changes depend strongly on the type and amplitude of the spanwise perturbation; it is the objective of this project to study this phenomenon computationally.

Vortex methods present natural candidates for the computations of highly concentrated regions of vorticity that evolve rapidly with time. We are constructing a three-dimensional time-dependent vortex simulation of a temporally developing mixing layer using a vortex-segment scheme. The scheme is designed to track the structure of elementary vortex elements in three dimensions using a combined Biot-Savart velocity calculation and a numerical implementation of the Kelvin-Helmholtz theorems on the transport of vorticity. The scheme maintains the advantage of two-dimensional vortex methods. Numerically, it provides a Lagrangian grid-free adaptive scheme with high resolution around areas of high concentration of vorticity. Physically, it ensures low levels of numerical diffusion by executing the transport of vorticity by convection in a Lagrangian frame of reference, hence allowing the growth of perturbations under unstable conditions.

The scheme is computationally-intensive and requires a large computer budget in terms of time and storage. This is due to two factors: (1) the mutual interactions among vortex segments, which is $O(N^2)$ where N is the number of vortex segments; (2) the satisfaction of the potential boundary conditions which amount to taking into consideration a large number of image vortices since conformal mapping methods do not apply in three dimensions.

We are currently working on the formulation and implementation of a Lagrangian-Eulerian scheme that utilizes fast and efficient scheme to solve the Laplace equation to compute the irrotational component of the velocity field on a grid while it preserves the Lagrangian nature of the calculations of vorticity transport. Employing a grid to solve for the potential component of the velocity does not endanger the non-diffusive nature of the overall method since this component does not possess sharp gradients within the field.

Preliminary application of this method indicates that the large-scale eddy structures that form as a result of the roll-up of the spanwise vorticity can sustain high amplitude spanwise perturbations. However, the rate of growth of the layer in the streamwise direction changes according to the type and relative size of this perturbation. Further studies are planned to identify various modes of instability, its effect on entrainment and mixing, and comparisons of the numerical predictions with experimental results. In particular, we are planning to monitor the formation of spanwise, mushroom-like structures and the migration of spanwise vorticity into the streamwise direction that has been observed experimentally (Ghoniem, Heidarinejad, and Ali [7]).

IV. Flame Propagation at Low Mach Numbers

The governing equations of turbulent combustion interactions were developed in Ghoniem, Chorin and Oppenheim*, based on the assumptions that (1) combustion occurs at constant pressure; (2) the flame structure is thin compared to the characteristic flow length; and (3) the laminar burning speed is constant, and independent of the flame surface topology. While this system is adequate for stable, constant burning speed flames that propagate in open channels, it is necessary to derive a new system that describes combustion in confined volumes where temporal pressure changes can give rise to an extra dynamic field, and when the self-turbulization of the flame is important to the dynamics of the flow field. This general system should allow the flame structure to affect its burning speed via the geometrical properties of its surface and the local properties of the reacting mixture, while maintaining desirable properties for numerical solutions.

Starting from the basic conservation equations for a two-component reacting mixture, we take the asymptotic limit at low Mach number, thus removing the effect of acoustic waves in situations where combustion generated velocities are much smaller than the local speed of sound. The resulting equations retain the effect of large density gradients, however, they are devoid of the sharp spatial gradients associated with sound waves, making their numerical integration easier and more efficient without sacrificing the essential physics. This system also allows transport properties and chemical kinetics, as well as the geometry of the enclosure and heat transfer across its surface, to affect the flame structure and its speed of burning. Next, we take the asymptotic limit for high activation

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*Phil. Trans. Roy. Soc. Lond., A304 (1982), pp. 303-325.

energy and small flame thickness to reduce the flame structure into a thin interface separating reactants and products.

The numerical scheme which will be used to solve for flame propagation in a turbulent environment is described in Ghoniem [7]. We are currently applying the model to study flame propagation and stability in a confined volume, resembling a combustion chamber of an engine. Preliminary results indicate that the numerical solution for a thin flame propagating at a constant burning speed agrees very accurately with the analytical solution of the same problem (Ghoniem [1]). This comparison will be employed to optimized the numerical parameters. We are planning to extend the application of the model to solve for cases of unsteady flame propagation in combustion chambers for which experimental data are available (Ghoniem and Knio [8]).

PUBLICATIONS

1. Ghoniem, A.F., "Computational methods in turbulent reacting flow," The 17th AMS-SIAM Summer Seminar in Applied Mathematics, Cornell University, Ithaca, N.Y., July 1985, to appear in Lectures in Applied Mathematics.

2. Ng, K.K. and Ghoniem, A.F., "Vortex simulation of a confined shear layer," The 10th International Colloquium on Dynamics of Explosions and Reactive Systems, Berkeley, CA, August 1985, to appear in Proceedings.

3. Ng, K.K. and Ghoniem, A.F., "Harmonic modulation of a confined shear layer," AIAA-86-0056, The 24th AIAA Aerospace Sciences Meeting, Reno, NV, January 1986.

4. Ghoniem, A.F. and Sethian, J.A., "Dynamics of turbulent structures in a recirculating flow; a computational study," AIAA-85-0146, submitted for publication to the AIAA Journal.

5. Gagnon, Y. and Ghoniem, A.F., "Low frequency oscillation of recirculating flow at low Reynolds number," AIAA-86-0370, The 24th AIAA Aerospace Sciences Meeting, Reno, NV, January 1986.

6. Ghoniem, A.F., "Analysis of flame deformation in a turbulent field; effect of Reynolds number on burning rates," AIAA-85-0140, submitted for publication to Comb. Flame.

7. Ghoniem, A.F., Heidarinejad, G., and Aly, H.F. "Two and three dimensional instabilities of a turbulent shear layer," in progress.

8. Ghoniem, A.F., and Knio, O. "Hydrodynamic instability of flames and the development of tulip-shaped structures," in progress.

PRESENTATIONS

1. "Development and Applications of Vortex Methods: Aerodynamics and Combustion," NASA Lewis Research Center, Cleveland, Ohio, June 1984.

2. "Simulation of a Turbulent Flow in a Model Combustor," 1984 Technical Meeting, Eastern Section of the Combustion Institute, Clearwater Beach, FA, December 1984.

3. "Flame propagation and stability in engine chambers," Department of Energy sponsored program on "Lean Engine Efficiency," Ford Motor Company, May 1985.

4. "Numerical solution of a confined shear layer using vortex methods," The International Symposium on Computational Fluid Dynamics, Tokyo, Japan, September 1985.

5. "Vortex Simulation of Turbulent Reacting Flow," AFSOR/ONR Contractors Meeting on Turbulent Combustion, July 1985.

6. "Application of Computational Methods in Turbulent Reacting Flow," University of North Carolina, October 1985.

7. "Vortex Simulation of Reacting Shear Flows," Army Research Office, Durham, North Carolina, October 1985.

INTERACTIONS

1. Participated in DOD meeting on Topical Review on Mechanics, Aeronautics and Propulsion, National Academy of Sciences, February 5-6, 1985.

2. NASA Lewis Research Center, Combustion Fundamentals (Dr. C. John Marek) and Computational Fluid Mechanics (Dr. John Adamczyk), June 1984.

3. California Institute of Technology, Combustion Laboratory of Prof. E. Zukoski, to explore their experimental work on pressure oscillations in dump combustors and couple to our numerical studies, July 1985.

4. Army Research Office, Mathematical Sciences Division (Dr. J. Chandra) (to visit the Laboratory on October 4, 1985, and explore avenues for interactions).

5. Pennsylvania State University, Combustion Laboratory of Dr. Dominic Santavicca, to couple his experimental investigation on the effect of turbulence on flame propagation (supported by AFOSR) to our numerical simulation activities (to visit the Laboratory on November 6th).

6. Sandia National Laboratory, couple experimental work on flame structure (Dr. R. Green) and engine efficiency (Dr. F. Dyer) with our numerical simulation studies.

7. Columbia University, N.Y., Combustion Laboratory of Drs. R. Bill and R. Chevery, to couple their experimental work on stability of V-shaped flames and axi-symmetric shear layers to our numerical simulations (to visit during this academic year, 1985-1986).

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